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6. AUTHOR(S)
DONALD S. COHEN

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, ca 91125

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Work has continued in two simultaneous veins. (1) Models have been developed to attempt to realistically account for recent observations involving new classes of polymerpenetrant systems. The attempt has been to account for their properties as they are currently being used in certain emerging technologies such as novel pharmaceutical delivery systems and separating membranes. (2) Since most of the new observations involve various aspects of non-Fickian diffusion coupled with viscoelastic mechanical properties, the mathematical models usually involve degenerate parabolic systems which give rise to new and fascinating types of mathematical behavior. They have provided the impetus to develop interesting analytical and numerical techniques.

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CALIFORNIA INSTITUTE OF TECHNOLOGY

APPLIED MATHEMATICS 217-50
FIRESTONE LABORATORY

May 10, 1991

Dr. Arje Nachman
Air Force Office of Scientific Research
Building 410
Bolling Air Force Base, D.C. 20332-6448

Dear Arje:

Final Technical Report
Air Force Grant AFOSR-88-0269
1 August 1988 - 31 July 1990

Work has continued in two simultaneous veins. (1) Models have been developed to attempt to realistically account for recent observations involving new classes of polymer-penetrant systems. The attempt has been to account for their properties as they are currently being used in certain emerging technologies such as novel pharmaceutical delivery systems and separating membranes. (2) Since most of the new observations involve various aspects of non-Fickian diffusion coupled with viscoelastic mechanical properties, the mathematical models usually involve degenerate parabolic systems which give rise to new and fascinating types of mathematical behavior. They have provided the impetus to develop interesting analytical and numerical techniques.

Professor Christopher Durning, a chemical engineering who is primarily an experimentalist, Dr. Andrew White, an applied mathematician who is primarily an expert in numerical methods, and I started a joint collaboration in the summer of 1990 when we met at Los Alamos to discuss and plan future research. We feel that genuine progress has been made in several directions under support of the AFOSR grant from 1988 to 1990.

PASADENA, CALIFORNIA 91125

This has been published and documented in the theses and publications list appended. The work has been well received and I have been asked to speak on it at many meetings and institutions. I am particularly excited that in the near future Professor Durning will carry out experiments to both test the new models and provided appropriate data to allow further realistic modelling.

Sincerely yours,

Don

Donald S. Cohen
Professor and Executive Officer
for Applied Mathematics

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enclosures

cc: Contracting Officer (AFOSR) w/enc.
Sponsored Research/CIT
Edward O. Ansell/CIT

Theses Abstracts

Diffusion and Stress Driven Flow in Polymers

Catherine Kent Hayes
California Institute of Technology

A recently proposed model for non-Fickian diffusion of penetrants into polymers is adapted and used to study a drug-delivery problem. The model modifies Fick's diffusion equation by the addition of stress-induced flux and a bimolecular reaction term. A stress evolution equation incorporating aspects of the Maxwell and Kelvin-Voigt viscoelastic stress models completes the model. The diffusivity and relaxation time in the polymer are taken as functions of the penetrant concentration.

The system is first studied on a doubly infinite domain under the assumption that the penetrant's saturation concentration is small. When the diffusivity and relaxation time are taken to be constant, a perturbation analysis is used to show the form and the region of stability of traveling-wave solutions. When the diffusivity and relaxation time are taken as specified functions of the concentration, the shapes of traveling-wave solutions are predicted by perturbation analysis and found to be different when the equations are diffusion-driven than when they are stress-driven. The predictions are verified by numerical integration for specified parameter values.

The system is also studied on a finite domain under the assumption that the diffusivity is large. A perturbation analysis is used to demonstrate that the concentration and stress evolve according to a Fickian diffusion equation on a short time scale. After longer time has elapsed, the concentration and stress are shown to exhibit steep fronts in a narrow region within the domain. These predictions are verified numerically. Finally, the equations are studied in the steady state and are found to predict the evolution of shocks.

Work done on Fisher's equation is presented in an appendix. When the diffusivity is taken in the same nonlinear form as was used in the polymer-penetrant model, a qualitatively new solution of Fisher's equation is found, using a method which is also applied to the polymer-penetrant system.

Asymptotic Methods in Semiconductor Device Modeling

Michael Jeffrey Ward
California Institute of Technology

The behavior of metal oxide semiconductor field effect transistors (MOSFETs) with small aspect ratio and large doping levels is analyzed using formal perturbation techniques. Formally, we will show that in the limit of small aspect ratio there is a region in the middle of the channel under the control of the gate where the potential is one-dimensional. The influence of interface and internal layers in the one-dimensional potential on the averaged channel conductivity is closely examined in the large doping limit. The interface and internal layers that occur in the one-dimensional potential are resolved in the limit of large doping using the method of matched asymptotic expansions. The asymptotic potential in the middle of the channel is constructed for various classes of variable doping models including a simple doping model for the built-in channel device. Using the asymptotic one-dimensional potential, the asymptotic mobile charge, needed for the derivation of the long-channel I-V curves, is found by using standard techniques in the asymptotic evaluation of integrals. The formal asymptotic approach adopted not only provides a pointwise description of the state variables, but by using the asymptotic mobile charge, the lumped long-channel current-voltage relations, which vary uniformly across the various bias regimes, can be found for various classes of variable doping models.

Using the explicit solutions of some free boundary problems solved by Howison and King (1988), the two-dimensional equilibrium potential near the source and drain is constructed asymptotically in strong inversion in the limit of large doping. From the asymptotic potential constructed near the source and drain, a uniform analytical expression for the mobile charge valid throughout the channel is obtained. From this uniform expression for the mobile charge, we will show how it is possible to find the I-V curve in a particular bias regime taking into account the edge effects of the source and drain. In addition, the asymptotic potential for a two-dimensional n^{+}-p junction is constructed.

Scientific Collaborators

Professor Christopher Durning
Department Chemical Engineering
Columbia University
New York, NY 10027

Professor Thomas Erneux
Department of Engineering Sciences
and Applied Mathematics
The Technological Institute
Northwestern Unviersity
Evanston, IL 60208

Dr. Andrew B. White
Los Alamos National Laboratory
MS265, P.O. Box 1663
Los Alamos, NM 87545

Graduate Students

3

Catherine Kent Hayes
Michael Jeffrey Ward

Publications

69. Sharp fronts due to diffusion and stress at the glass transition in polymers, J. Polymer Science B: Polymer Physics, 27 (1989) 1731-1741; (with A.B. White).

70. Delayed diffusion due to flux limitation, Physics Letters A, 142 (1989) 26-30; (with P. Rosenau, P.S. Hagan, and R.L. Northcutt).

71. Changing time history in moving boundary problems, SIAM J. Appl. Math., 50 (1990) 483-489; (with T. Erneux).

72. Asymptotic methods for metal oxide semiconductor field effect transistor modeling, SIAM J. Appl. Math., 50 (1990) 1099-1125; (with M.J. Ward and F.M. Odeh).

Manuscripts In Preparation

73. Sharp fronts due to diffusion and viscoelastic relaxation in polymers, SIAM J. Appl. Math, to appear (with A.B. White).

74. The evolution of steep fronts in non-Fickian polymer-penetrant systems, J. Polymer Science B: Polymer Physics, to appear (with C.K. Hayes).

75. Stress assisted and stress impeded diffusion: moving and stopping fronts, SIAM J. Appl. Math., to appear (with A.B. White).